Appendix B

Applicants : Keith P. Wilson et al. Docket No.: VPI/96-03 DIV2
Application No. : 09/678,016 Filed : October 2, 2000
For : MOLECULES COMPRISING AN IMPDH-LIKE BINDING POCKET AND
ENCODED DATA STORAGE MEDIUM CAPABLE OF GRAPHICALLY
DISPLAYING THEM

Attorney: James F. Haley, Jr. Reg. No. 27,794 Tel: (212) 596-9000 Sheet 34/118

## FIG. 1A-34

	-								
ATOM	1945	CA	GLY	324	69.392	74.347	78.362	1.00	13.80
ATOM	1946	С	GLY	324	68.211	75.201	78.791	1.00	14.53
ATOM	1947	0	GLY	324	68.367	76.397	78.997	1.00	17.39
ATOM	1948	Ν	MET	325	67.026	74.613	78.901	1.00	11.83
ATOM	1949	CA	MET	325	65.868	75.368	79.341	1.00	13.08
ATOM	1950	CB	MET	325	65.201	76.124	78.186	1.00	12.41
ATOM	1951	CG	MET	325	64.150	77.118	78.678	1.00	10.52
ATOM	1952	SD	MET	325	63.227	78.025	77.440	1.00	13.36
ATOM	1953	CE	MET	325	62.495	79.307	78.488	1.00	7.16
ATOM	1954	С	MET	325	64.829	74.561	80.130	1.00	15.26
ATOM	1955	0	MET	325	64.051	73.781	79.563	1.00	15.50
ATOM	1956	Ν	GLY	326	64.848	74.751	81.447	1.00	15.85
ATOM	1957	CA	GLY	326	63.899	74.093	82.323	1.00	17.08
ATOM	1958	С	GLY	326	64.165	72.651	82.677	1.00	18.22
ATOM	1959	.0	GLY	326	63.270	71.957	83.148	1.00	18.82
ATOM	1960	Ν	CYS	327	65.401	72.206	82.515	1.00	20.56
ATOM	1961	CA	CYS	327	65.746	70.823	82.821	1.00	22.33
ATOM	1962	CB	CYS	327	66.443	··· 70.194	81.622	1.00	20.50
ATOM	1963	SG	CYS	327	67.878	71.121	81.089	1.00	ູ 21.45
ATOM	1964	С	CYS	327	66.633	70.710	84.061	1.00	24.86
ATOM	1965	0	CYS	327	66.992	69.597	84.487	1.00	26.55
ATOM	1966	N	GLY	328	67.007	71.859	84.619	1.00	23.64
ATOM	1967	CA	GLY	328	67.846	71.867	85.802	1.00	23.90
ATOM	1968	C	GLY	328	67.066	71.347	86.988	1.00	23.07
ATOM	1969	0	GLY	328	65.913	71.735	87.168	1.00	23.22
ATOM	1970	N	SER	329	67.706	70.528	87.822	1.00	23.68
ATOM	1971	CA	SER	329	67.077	69.925	89.000	1.00	22.19
ATOM	1972	СВ	SER	329	68.150	69.406	89.964	1.00	19.55
ATOM	1973	ŌĞ	SER	329	69.028	70.440	90.356	1.00	23.14
ATOM	1974	C	SER	329	66.077	70.812	89.747	1.00	23.28
ATOM	1975	Ö	SER	329	64.978	70.362	90.065	1.00	25.72
ATOM	1976	Ñ	ILE	330	66.444	72.070	89.992	1.00	22.81
ATOM	1977	CA	ILE	330	65.584	73.024	90.700	1.00	19.85
ATOM	1978	CB	ILE	330	66.410	74.017	91.589	1.00	15.67
ATOM	1979	CG2	ILE	330	66.509	73.500	93.001	1.00	18.25
ATOM	1980	CG1	ILE	330	67.795	74.289	90.994	1.00	7.11
ATOM	1981	CD1	ILE	330	67.776	74.921	89.639	1.00	5.46
ATOM	1982	С	ILE	330	64.703	73.869	89.786	1.00	20.60
ATOM	1983	0	ILE	330	64.225	74.923	90.201	1.00	23.53
ATOM	1984	N	IMP	331	64.425	73.400	88.579	1.00	19.32
ATOM	1985	CA	IMP	331	63.641	74.206	87.649	1.00	20.33
ATOM	1986	С	IMP	331	62.148	73.909	87.498	1.00	21.39
ATOM	1987	0	IMP	331	61.737	72.757	87.342	1.00	22.62
ATOM	1988	CB	IMP	331	64.310	74.200	86.277	1.00	19.26
ATOM	1989	SG	IMP	331	64.038	75.775	85.516	1.00	16.83
ATOM	1990	Р	IMP	331	71.205	71.206	87.339	1.00	24.40
ATOM	1991	O1P	IMP	331	70.381	70.028	86.885	1.00	22.40
ATOM	1992	O2P	IMP	331	72.615	71.144	86.864	1.00	18.66
ATOM	1993	O3P	IMP	331	71.172	71.333	88.803	1.00	19.75
ATOM	1994	O5*	IMP.	331	70.688	72.534	86.798	1.00	22.96
ATOM	1995	C5*	IMP	331	71.500	73.726	87.024	1.00	14.95
ATOM	1996	C4*	IMP	331	71.156	74.601	85.831	1.00	11.32
ATOM	1997	04*	IMP	331	69.758	74.898	85.861	1.00	12.20
ATOM	1998	C3*	IMP	331	71.865	75.962	85.934	1.00	12.62
ATOM	1999	O3*	IMP	331	73.078	76.011	85.208	1.00	10.24
ATOM	2000	C2*	IMP	331	70.883	76.903	85.210	1.00	13.74
ATOM	2001	02*	IMP	331	70.752	76.706	83.816	1.00	11.66
ATOM	2002	C1*	IMP	331	69.602	76.308	85.761	1.00	14.52
ATOM	2003	N9	IMP	331	68.832	77.205	86.612	1.00	18.13

Applicants : Keith P. Wilson et al. Docket No.: VPI/96-03 DIV2
Application No. : 09/678,016 Filed : October 2, 2000
For : MOLECULES COMPRISING AN IMPDH-LIKE BINDING POCKET
AND ENCODED DATA STORAGE MEDIUM CAPABLE OF
GRAPHICALLY DISPLAYING THEM
Attorney: James F. Haley, Jr. Reg. No. 27,794 Tel: (212) 596-9000 Sheet 35/118

## FIG. 1A-35

					FIG. IA-3	3			
ATOM	2004	C8	IMP	331	69.321	78.030	87.599	1.00	18.02
ATOM	2005	N7	IMP	331	68.331	78.568	88.322	1.00	16.06
ATOM	2006	C5	IMP	331	67.170	78.093	87.806	1.00	19.77
ATOM	2007	C6	IMP	331	65.799	78.289	88.156	1.00	22.26
ATOM	2008	06	IMP	331	65.412	78.995	89.085	1.00	17.37
ATOM	2009	N1	IMP	331	64.941	77.579	87.374	1.00	25.96
ATOM	2010	C2	IMP	331	65.296	76.706	86.299	1.00	23.29
ATOM	2011	N3	IMP	331	66.567	76.524	85.957	1.00	24.20
ATOM	2012	C4	IMP	331	67.498	77.200	86.693	1.00	21.15
ATOM	2013	N	ILE	332	61.333	74.959	87.564	1.00	19.04
ATOM	2014	CA.	ILE	332	59.899	74.811	87.391	1.00	18.02
ATOM	2015	CB	ILE	332	59.071	75.097	88.696	1.00	16.99
ATOM	2016	CG2	ILE	332	59.423	74.093	89.793	1.00	12.90
ATOM	2017	CG1	ILE	332	59.283	76.525	89.191	1.00	14.79
ATOM	2017	CD1	ILE	332	58.212	77.005	90.159	1.00	8.04
ATOM	2019	C	ILE	332	59.401	77.675 75.675	86.226	1.00	20.21
ATOM	2019	Ö	ILE	332	58.195	75.848	86.050	1.00	21.52
ATOM	2020	N	THR	333	60.330	76.195	85.420	1.00	20.15
				333	59.993	77.020	84.251	1.00	19.79
ATOM	2022	CA	THR			77.491	83.467	1.00	20.47
ATOM	2023	CB OC4	THR	333	61.287	77.491 78.537	84.191	1.00	18.21
ATOM	2024	OG1	THR	333	61.948			1.00	16.88
ATOM	2025	CG2	THR	333	60.949	77.996	82.058	1.00	18.99
ATOM	2026	C	THR	333	59.060	76.275	83.281		19.34
ATOM	2027	0	THR	333	58.124	76.861	82.737	1.00	16.88
ATOM	2028	N	GLN	334	59.308	74.988	83.063	1.00	
ATOM	2029	CA	GLN	334	58.469	74.229	82.150	1.00	16.64
ATOM	2030	CB	GLN.	334	59.077	72.850	81.863	1.00	15.49
ATOM	2031	CG	GLN	334	60.004	72.864	80.658	1.00	16.53
ATOM	2032	CD	GLN	334	60.874	71.628	80.536	1.00	18.34
ATOM	2033	OE1	GLN	334	62.091	71.729	80.344	1.00	16.42
ATOM	2034	NE2	GLN	334	60.257	70.461	80.604	1.00	20.90
ATOM	2035	C	GLN	334	57.046	74.122	82.667	1.00	16.88
ATOM	2036	0 .	GLN	334	56.091	74.293	81.916	1.00	15.78
ATOM	2037	N .	GLU	335	56.910	73.919	83.971	1.00	19.92
ATOM	2038	CA	GLU	335	55.596	73.795	84.583	1.00	21.69
ATOM	2039	CB	GLU	335	55.699	73.203	85.987	1.00	25.79
ATOM	2040	CG	GLU	335	56.398	71.865	86.047	1.00	32.28
ATOM	2041	CD	GLU	335	57.745	71.971	86.700	1.00	37.56
ATOM	2042	OE1	GLU	335	58.715	72.312	85.988	1.00	35.47
ATOM	2043	OE2	GLU	335	57.826	71.736	87.930	1.00	40.35 20.91
ATOM	2044	<b>C</b> .	GLU	335	54.878	75.123	84.675	1.00	23.86
ATOM	2045	0	GLU	335	53.680	75.192 70.470	84.440	1.00	
ATOM	2046	N	VAL	336	55.608	76.176	85.022	1.00	20.29
ATOM	2047	CA	VAL	336	55.003	77.488	85.167	1.00	18.99
ATOM	2048	CB	VAL	336	55.776	78.368	86.175	1.00	19.44
ATOM	2049	CG1	VAL	336	55.043	79.675	86.381	1.00	23.03
ATOM	2050	CG2	VAL	336	55.922	77.651	87.510	1.00	16.34
ATOM	2051	C	VAL	336	54.822	78.232	83.851	1.00	16.99
ATOM	2052	0	VAL	336	53.752	78.764	83.595	1.00	17.91
ATOM	2053	N	LEU	337	55.837	78.239	82.997	1.00	14.89
ATOM	2054	CA	LEU	337	55.720	78.960	81.732	1.00	15.59
ATOM	2055	CB	LEU	337	56.918	79.902	81.534	1.00	14.85
ATOM	2056	CG	LEU	337	57.263	80.856	82.688	1.00	13.73
ATOM	2057	CD1	LEU	337	58.394	81.763	82.271	1.00	14.07
ATOM	2058	CD2	LEU	337	56.062	81.687	83.108	1.00	13.59
ATOM	2059	С	LEU	337	55.468	78.133	80.467	1.00	14.97
ATOM	2060	0	LEU	337	55.399	78.690	79.371	1.00	16.68
ATOM	2061	N	ALA	338	55.386	76.812	80.599	1.00	12.41
ATOM	2062	CA	ALA	338	55.109	75.933	79.456	1.00	12.62